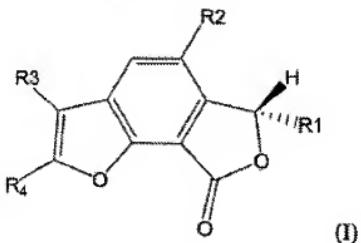


Claims

10/576758

1. Compounds of the general formula (I) and their derivatives



in which

R1 represents C_1 - C_4 alkyl;

R2 represents H, halogen, -OH, NRR' or $-NO_2$, wherein R and R' represent H or C_1 - C_6 alkyl;

R3 represents H, halogen, -OH, NRR' or $-NO_2$, wherein R and R' represent H or C_1 - C_6 alkyl;

R4 represents H, halogen or $-NO_2$.

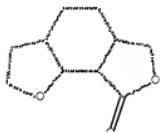
10/576758

***** INVENTOR RESULTS *****

=> d his 119

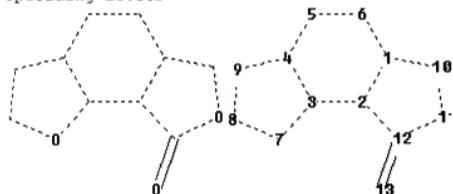
(FILE 'HCAPLUS' ENTERED AT 11:10:14 ON 12 DEC 2008)
L19 3 S ((L12-L18) AND L4) OR (L4 AND L8)

=> d que 119 L1 STR



Structure attributes must be viewed using STN Express query preparation:

Uploading L1.str



chain nodes :

13

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

12-13

ring bonds :

1-2 1-6 1-10 2-3 2-12 3-4 3-7 4-5 4-9 5-6 7-8 8-9 10-11 11-12

exact/norm bonds :

1-2 1-6 1-10 2-3 2-12 3-4 3-7 4-5 4-9 5-6 7-8 8-9 10-11 11-12 12-13

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS

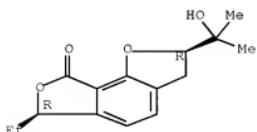
L3 52 SEA FILE=REGISTRY SSS FUL L1
L4 22 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

L8	1	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	US20070155830/PN
L12	50007	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	LIU J?/AU
L13	12465	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	ZHENG Y?/AU
L14	2276	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	QIN X?/AU
L15	15784	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	YANG L?/AU
L16	3525	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	DONG Z?/AU
L17	15567	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	WANG R?/AU
L18	3211	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	TAN J?/AU
L19	3	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	((L12 OR L13 OR L14 OR L15 OR L16 OR L17 OR L18) AND L4) OR (L4 AND L8)

==> d 119 1=3 ibib abs hitstr

L19 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2008:488982 HCAPLUS Full-text
 DOCUMENT NUMBER: 149173557
 TITLE: Induced daldinin A, B, C with a new skeleton from
 cultures of the ascomycete *Daldinia concentrica*
 AUTHOR(S): Shao, Hong-Jun; Qin, Xiang-Dong; Dong,
 Ze-Jun; Zhang, Hong-Bin; Liu, Ji-Kai
 CORPORATE SOURCE: State Key Laboratory of Phytochemistry and Plant
 Resources in West China, Kunming Institute of Botany,
 Chinese Academy of Sciences, Kunming, 650204, Peop.
 Rep. China
 SOURCE: Journal of Antibiotics (2008), 61(3), 115-119
 CODEN: JANTAJ; ISSN: 0021-8820
 PUBLISHER: Japan Antibiotics Research Association
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Daldinin A, B, C with a new skeleton, together with four known compds., were
 induced and isolated from cultures of the ascomycete *Daldinia concentrica*.
 Their structures were elucidated by spectroscopic anal., and that of daldinin
 A was confirmed by single-crystal x-ray diffraction.
 IT 1033349-51-7P, Daldinin B
 RL: BSU (Biological study, unclassified); NPO (Natural product
 occurrence); PRP (Properties); PUR (Purification or recovery); BIOL
 (Biological study); OCCU (Occurrence); PREP (Preparation)
 (induced daldinin A, B, C with new skeleton from cultures of ascomycete
Daldinia concentrica)
 RN 1033349-51-7 HCAPLUS
 CN Furo[2,3-e]isobenzofuran-8(2H)-one,
 6-ethyl-3,6-dihydro-2-(1-hydroxy-1-methylethyl)-, (2R,6R)-rel-(-)- (CA
 INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.
Currently available stereo shown.



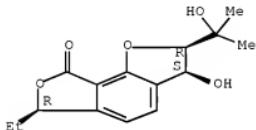
IT 10233349-49-3P, Daldinin A

RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation of from cultures of ascomycete *Daldinia concentrica* and crystal and mol. structure of)

RN 1033349-49-3 HCAPLUS

CN Furo[2,3-e]isobenzofuran-8(2H)-one,
6-ethyl-3,6-dihydro-3-hydroxy-2-(1-hydroxy-1-methylethyl)-,
(2R,3S,6R)-rel-(-) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.
Currently available stereo shown.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:121182 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 1441:346530

TITLE: Concentricolide, an anti-HIV agent from the ascomycete *Daldinia concentrica*

AUTHOR(S): Qin, Xiang-Dong; Dong, Ze-Jun;
Liu, Ji-Kai; Yang, Liu-Meng;
Wang, Rui-Rui; Zheng, Yong-Tang; Lu,
Yang; Wu, Yun-Shan; Zheng, Qi-Tai

CORPORATE SOURCE: State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming, 650204, Peop. Rep. China

SOURCE: Helvetica Chimica Acta (2006), 89(1), 127-133
CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal
LANGUAGE: English

AB A novel benzofuran lactone, named concentricolide (=rel-(6R)-6-ethylbenzo[2,1-b:3,4-c']difuran-8(6H)-one; 1), was isolated along with four known compds. (friedelin, cytochalasin L-696,474, armillaramide, and russulamide) from the fruiting bodies of the xylariaceous ascomycete *Daldinia concentrica*. The structure of 1 was established by spectroscopic methods and x-ray crystallog. anal. Its anti-HIV-1 activity was tested. Results showed that 1 inhibited HIV-1 induced cytopathic effects. The EC50 value was 0.31 µg/mL. The therapeutic index (TI) was 247. Concentricolide exhibited the blockage (EC50 0.83 µg/mL) on syncytium formation between HIV-1 infected cells and normal cells.

IT 850078-65-8P

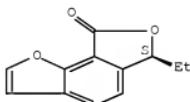
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological

study); OCCU (Occurrence); PREP (Preparation); USES (Uses)
 (isolation, purification, and characterization of concentricolide from
 ascomycete *Daldinia concentrica*)

RN 850078-65-8 HCPLUS

CN Furo[2,3-*e*]isobenzofuran-8(6H)-one, 6-ethyl-, (6*S*)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 3 OF 3 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:371265 HCPLUS Full-text

DOCUMENT NUMBER: 142:392220

TITLE: Preparation of Concentricolide and its derivatives and application as anti-HIV agent for pharmaceutical compositions

INVENTOR(S): Liu, Jikai; Zheng, Yongtang;
 Qin, Xiangdong; Yang, Liuemeng;
 Dong, Zejun; Wang, Ruirui; Tan,
 Jianwen

PATENT ASSIGNEE(S): Kunming Institute of Botany, the Chinese Academy of Sciences, Peop. Rep. China; Kunming Institute of Zoology, the Chinese Academy of Sciences

SOURCE: PCT Int. Appl., 31 pp.
 CODEN: PIXXD2

DOCUMENT TYPE: Patent

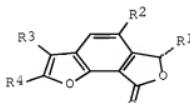
LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005037841	A1	20050428	WO 2004-CN1188	20041020
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CN 1537855	A	20041020	CN 2003-10110784	20031022
CN 1238357	C	20060125		
DE 112004002032	T5	20061005	DE 2004-112004002032	20041020
JP 2007509080	T	20070412	JP 2006-535929	20041020

US 20070155830 A1 20070705 US 2007-576758 20070305 <--
 PRIORITY APPLN. INFO.: CN 2003-10110784 A 20031022
 OTHER SOURCE(S): MARPAT 142:392220 W 20041020
 GI



I

AB Concentricolide and its derivs. I (R1 = C1-C4; R2 = H, halo, OH, NRR', R and R' = H, c1-c6 alkyl; R3 = H, halo, OH, NRR', NO2, R and R' = H, or C1-C6 alkyl; R4 = H, halo, NO2), are prepared from *Daldinia concentrica* via extraction with organic solvent to give Concentricolide A, further bromination, nitration, and alkylation to provide its derivs. Title compds. can be used as pharmaceutical compns. for treating and preventing the infection of human immunodeficiency virus (HIV).

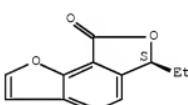
IT 850078-65-0P

RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PUR (Purification or recovery); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (preparation of Concentricolide A as anti-HIV agent)

RN 850078-65-8 HCPLUS

CN Furo[2,3-e]isobenzofuran-8(6H)-one, 6-ethyl-, (6S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

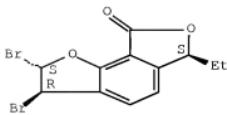
IT 850078-66-9P 850078-67-0P 850078-68-1P
 850078-69-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of Concentricolide as anti-HIV agent)

RN 850078-66-9 HCPLUS

CN Furo[2,3-e]isobenzofuran-8(2H)-one, 2,3-dibromo-6-ethyl-3,6-dihydro-, (2S,3R,6S)- (CA INDEX NAME)

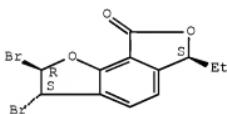
Absolute stereochemistry.



RN 850078-67-0 HCPLUS

CN Furo[2,3-e]isobenzofuran-8(2H)-one, 2,3-dibromo-6-ethyl-3,6-dihydro-, (2R,3S,6S)- (CA INDEX NAME)

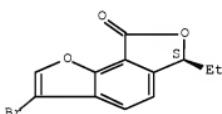
Absolute stereochemistry.



RN 850078-68-1 HCPLUS

CN Furo[2,3-e]isobenzofuran-8(6H)-one, 3-bromo-6-ethyl-, (6S)- (CA INDEX NAME)

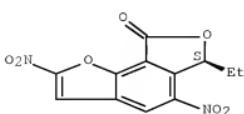
Absolute stereochemistry.



RN 850078-69-2 HCPLUS

CN Furo[2,3-e]isobenzofuran-8(6H)-one, 6-ethyl-2,5-dinitro-, (6S)- (CA INDEX NAME)

Absolute stereochemistry.



10/576758

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

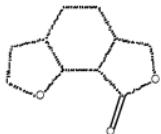
10/576758

***** QUERY RESULTS *****

=> d his 120

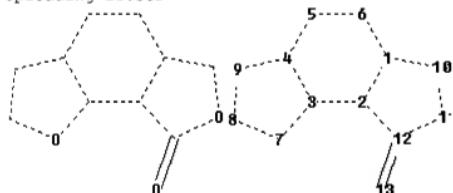
(FILE 'HCPLUS' ENTERED AT 11:10:14 ON 12 DEC 2008)
L20 19 S L4 NOT L19

=> d que 120
L1 STR



Structure attributes must be viewed using STN Express query preparation:

Uploading L1.str



chain nodes :

13

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

12-13

ring bonds :

1-2 1-6 1-10 2-3 2-12 3-4 3-7 4-5 4-9 5-6 7-8 8-9 10-11 11-12

exact/norm bonds :

1-2 1-6 1-10 2-3 2-12 3-4 3-7 4-5 4-9 5-6 7-8 8-9 10-11 11-12 12-13

isolated ring systems :

containing 1 :

Match level :

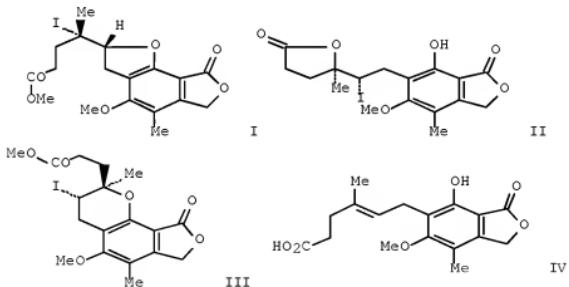
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS

L3 52 SEA FILE=REGISTRY SSS FUL L1

L4	22	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L3
L8	1	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	US20070155830/PN
L12	50007	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	LIU J?/AU
L13	12465	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	ZHENG Y?/AU
L14	2276	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	QIN X?/AU
L15	15784	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	YANG L?/AU
L16	3525	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	DONG Z?/AU
L17	15567	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	WANG R?/AU
L18	3211	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	TAN J?/AU
L19	3	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	((L12 OR L13 OR L14 OR L15 OR L16 OR L17 OR L18)) AND L4) OR (L4 AND L8)
L20	19	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L4 NOT L19

=> d 120 1-19 ibib abs hitstr hitind

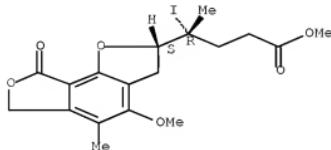
L20 ANSWER 1 OF 19 HCPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:600699 HCPLUS Full-text
DOCUMENT NUMBER: 148:308076
TITLE: The Stereo Structures of Some Mycophenolic Acid Derivatives
AUTHOR(S): Bernhardt, Paul V.; Carman, Raymond M.; Le, Tri T.
CORPORATE SOURCE: Department of Chemistry, University of Queensland, Brisbane, QLD 4072, Australia
SOURCE: Australian Journal of Chemistry (2007), 60(5), 354-357
CODEN: AJCHAS; ISSN: 0004-9425
PUBLISHER: CSIRO Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:308076
GI



AB The mol. structure and configuration of three iodo compds. I, II and III, derived from mycophenolic acid (IV), were determined by X-ray crystallog.
IT 66341-98-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

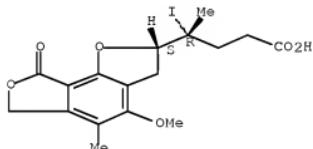
(synthesis and crystal structure of mycophenolic acid iodo derivs.)
 RN 66341-96-6 HCAPLUS
 CN Benzo[2,1-b:3,4-c']difuran-2-butanoic acid,
 2,3,6,8-tetrahydro- γ -iodo-4-methoxy- γ ,5-dimethyl-8-oxo-,
 methyl ester, (γ R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.

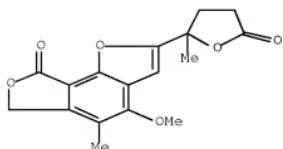


IT 66341-95-5P 66342-09-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (synthesis and crystal structure of mycophenolic acid iodo derivs.)
 RN 66341-95-5 HCAPLUS
 CN Benzo[2,1-b:3,4-c']difuran-2-butanoic acid,
 2,3,6,8-tetrahydro- γ -iodo-4-methoxy- γ ,5-dimethyl-8-oxo-,
 (γ R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 66342-09-4 HCAPLUS
 CN Furo[2,3-e]isobenzofuran-8(6H)-one,
 4-methoxy-5-methyl-2-(tetrahydro-2-methyl-5-oxo-2-furanyl)- (CA INDEX
 NAME)



CC 26-6 (Biomolecules and Their Synthetic Analogs)
 Section cross-reference(s): 75
 IT 66341-91-1P 66341-96-6P 66341-98-8P 959326-75-1P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (synthesis and crystal structure of mycophenolic acid iodo derivs.)
 IT 66341-95-5P 66342-09-4P 1009565-31-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (synthesis and crystal structure of mycophenolic acid iodo derivs.)
 REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 2 OF 19 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 20061924493 HCPLUS Full-text
 DOCUMENT NUMBER: 146:184386
 TITLE: Intramolecular cycloaddition reaction of bromo- and
 nitro-substituted furanyl amides
 AUTHOR(S): Padwa, Albert; Crawford, Kenneth R.; Straub,
 Christopher S.
 CORPORATE SOURCE: Department of Chemistry, Emory University, Atlanta,
 GA, 30322, USA
 SOURCE: ARKIVOC (Gainesville, FL, United States) (2007), (8),
 14-25
 CODEN: AGFUAR
 URL: [http://www.arkat-](http://www.arkat-usa.org/ARKIVOC/JOURNAL_CONTENT/manuscripts/2007/WA-1982AP%20as%20published%20mainmanuscript.pdf)
 usa.org/ARKIVOC/JOURNAL_CONTENT/manuscripts/2007/WA-
 1982AP%20as%20published%20mainmanuscript.pdf
 PUBLISHER: Arkat USA Inc.
 DOCUMENT TYPE: Journal; (online computer file)
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 146:184386
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

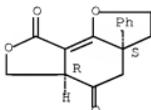
AB The intramol. Diels-Alder reaction (IMDAF) of an N-alkenyl-substituted furanyl amide (I, X = H) was investigated. Upon thermolysis at 80-110°, a smooth IMDAF reaction occurred to provide a stable aza-7-oxabicyclo[2.2.1]heptane cycloadduct (II) in high yield. The intramol. cyclization of the related 5-bromo-substituted furanyl amide (I, X = Br) was found to proceed at a much faster rate and in higher yield than the unsubstituted variant. The rate enhancement observed by incorporating a bromine in the 5-position of the furan ring appears to be general. The origin of the increased rate of cycloaddn. for the 5-bromo-substituted furan when compared to the unsubstituted example can be attributed to an increase in reaction exothermicity; this both decreases the activation enthalpy and increases the barrier to retrocycloaddn. Bromine substitution on furan also increases reactant energy and stabilizes the product due to the preference of the electroneg. bromine atom to be attached to a more highly alkylated, and therefore more electropos., framework. An unusual isomerization-cyclization reaction of a 5-nitro-substituted furanyl amide (III) was also found to occur, under microwave conditions, and provided a dihydrobenzofuropyrindine derivative (IV).
 IT 289673-97-8P 289673-98-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)

(intramol. Diels-Alder reaction of furan derivs.)

RN 289673-97-8 HCPLUS

CN Furo[2,3-e]isobenzofuran-5,8-dione, 2,3,3a,4,5a,6-hexahydro-3a-phenyl-, (3aR,5aS)-rel- (CA INDEX NAME)

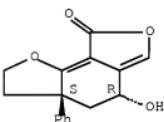
Relative stereochemistry.



RN 289673-98-9 HCPLUS

CN Furo[2,3-e]isobenzofuran-8(2H)-one, 3,3a,4,5-tetrahydro-5-hydroxy-3a-phenyl-, (3aR,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.



CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 289673-97-8P 289673-98-9P 583052-88-4P 583053-07-0P

906344-83-0P 906344-86-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(intramol. Diels-Alder reaction of furan derivs.)

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 3 OF 19 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:530448 HCPLUS [Full-text](#)

DOCUMENT NUMBER: 145:210776

TITLE: Use of Benzofuran for Concomitant Protection of Aldehyde and Phenol Groups in the Preparation of Mycophenolic Acid Analogues

AUTHOR(S): Fardis, Maria; Mertzman, Michael; Thomas, William; Kirschberg, Thorsten; Collins, Nicole; Polniaszek, Richard; Watkins, William J.

CORPORATE SOURCE: Gilead Sciences, Foster City, CA, 94404, USA
SOURCE: Journal of Organic Chemistry (2006), 71(13), 4835-4839

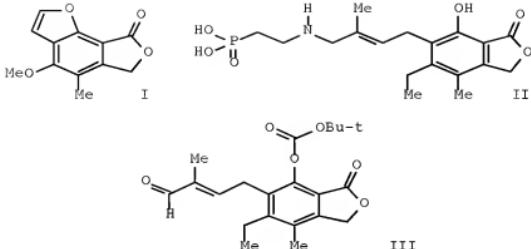
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:210776

GI



AB The use of a benzofuran to mask phenol and arylacetraldehyde moieties simultaneously in the synthesis of analogs of mycophenolic acid (MPA) was explored. Benzofuran I provided a stable and easily handled intermediate for the preparation of unnatural derivs. at the C-6 position of MPA. Preparation of the highly potent 6-Et MPA analog II was accomplished via aldehyde III through this facile route with high-yielding steps and crystalline intermediates.

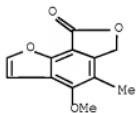
IT 903876-22-3P 903876-23-3P 903876-24-4P
903876-25-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of mycophenolic acid analogs via use of benzofuran as protection of aldehyde and phenol groups)

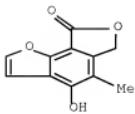
RN 903876-22-2 HCAPLUS

CN Euro[2,3-*e*]isobenzofuran-8(6H)-one, 4-methoxy-5-methyl- (CA INDEX NAME)

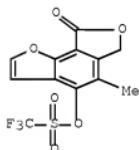


RN 903876-23-3 HCAPLUS

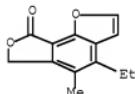
CN Euro[2,3-*e*]isobenzofuran-8(6H)-one, 4-hydroxy-5-methyl- (CA INDEX NAME)



RN 903876-24-4 HCAPLUS
 CN Methanesulfonic acid, 1,1,1-trifluoro-,
 6,8-dihydro-5-methyl-8-oxofuro[2,3-e]isobenzofuran-4-yl ester (CA INDEX
 NAME)



RN 903876-25-5 HCAPLUS
 CN Furo[2,3-e]isobenzofuran-8(6H)-one, 4-ethyl-5-methyl- (CA INDEX NAME)



CC 26-6 (Biomolecules and Their Synthetic Analogs)
 IT 24953-96-6P 903876-22-2P 903876-23-3P
 903876-24-4P 903876-25-5P 903876-26-6P 903876-27-7P
 903876-28-8P 903876-29-9P 903876-30-2P 903876-31-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of mycophenolic acid analogs via use of benzofuran as
 protection of aldehyde and phenol groups)
 REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 4 OF 19 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2006:499106 HCAPLUS Full-text
 DOCUMENT NUMBER: 145:166993
 TITLE: Phosphonic acid-containing analogs of mycophenolic
 acid as inhibitors of IMPDH
 Watkins, William J.; Chen, James M.; Cho, Aesop;
 Chong, Lee; Collins, Nicole; Fardis, Maria; Huang,

Wei; Hung, Magdeleine; Kirschberg, Thorsten; Lee, William A.; Liu, Xiaohong; Thomas, William; Xu, Jie; Zeynalzadegan, Ameneh; Zhang, Jennifer

CORPORATE SOURCE: Gilead Sciences, Inc., Foster City, CA, 94404, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2006),
 16(13), 3479-3483

CODEN: BMCLE8; ISSN: 0960-894X

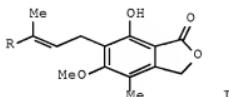
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:166993

GI



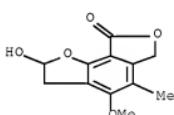
AB The design, synthesis, and IMPDH inhibitory activity of a series of phosphonic acid-containing analogs, such as I [R = XPO3H2, X = linking group, such as CH2, (CH2)2, (CH2)3, CH2OCH2, CH:CH, CH2NHCH2, (CH2)2NHCH2, (CH2)2N(COMe)CH2, (CH2)2N(CHO)CH2, (CH2)2N(SO2Me)CH2], of mycophenolic acid I [R = (CH2)2CO2H] were described.

IT 402731-00-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (phosphonic acid-containing analogs of mycophenolic acid as inhibitors of IMPDH)

RN 402731-00-4 HCPLUS

CN Furo[2,3-e]isobenzofuran-8(2H)-one,
 3,6-dihydro-2-hydroxy-4-methoxy-5-methyl- (CA INDEX NAME)



CC 26-6 (Biomolecules and Their Synthetic Analogs)

Section cross-reference(s): 1, 7

IT 24280-92-0P 31327-49-8P 402731-00-4P 402731-02-6P

790701-36-9P 790701-48-3P 790701-52-9P 790702-68-0P 790703-37-6P

790703-46-7P 790703-66-1P 790703-76-3P 900865-64-7P 900865-65-8P

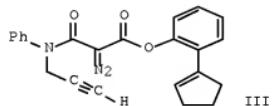
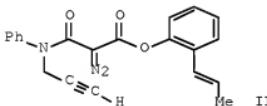
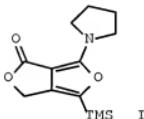
900865-66-9P 900865-67-0P 900865-68-1P 900865-69-2P 900865-70-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(phosphonic acid-containing analogs of mycophenolic acid as inhibitors of IMPDH)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 5 OF 19 HCPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:943377 HCPLUS Full-text
DOCUMENT NUMBER: 138:170018
TITLE: Synthesis of furo[3,4-c]furans using a
rhodium(II)-catalyzed cyclization/Diels-Alder
cycloaddition sequence
AUTHOR(S): Padwa, Albert; Straub, Christopher S.
CORPORATE SOURCE: Department of Chemistry, Emory University, Atlanta,
GA, 30322, USA
SOURCE: Journal of Organic Chemistry (2003), 68(2), 227-239
CODEN: JOCCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:170018
GI



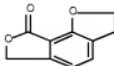
AB A series of 2-alkynyl 2-diazomalonates, when treated with a catalytic quantity of rhodium(II) acetate, afforded furo[3,4-c]furans, e.g., I, in good yield. The reaction proceeds by addition of a rhodium-stabilized carbеноид onto the acetylenic π -bond to give a vinyl carbеноид that subsequently cyclizes onto the neighboring carbonyl group to produce the furan ring. These furo[3,4-c]furans react with various dienophiles, furnishing anisole derivs. derived by loss of water from the initially formed Diels-Alder cycloadducts. The Rh(II)-catalyzed cyclization reaction was quite versatile with regard to the nature of the interacting carbonyl group. The methodol. was applied to the synthesis of several oxa-polyheterocyclic systems by first generating a 2-alkoxy-substituted furan and then allowing it to undergo a subsequent intramol. Diels-Alder cycloaddn. Ring opening of the resulting cycloadduct is followed by deprotonation to furnish a rearranged keto lactone. The potential use of this method for the synthesis of the alkaloid strychnine was probed using suitable model diazo compds. To establish the viability of this approach, the Rh(II)-catalyzed cyclization/cycloaddn. sequence of α -diazo amides II and III were studied. Both compds. underwent the sequential process in good overall yield, leading to novel pentacyclic products. The structural features of the resultant products present numerous opportunities for postcycloaddn. manipulations that could be exploited to synthetic advantage.

IT 289673-95-6P 289673-96-7P 289673-97-8P
289673-98-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of polycyclic furans via rhodium catalyzed
cyclization/Diels-Alder cycloaddn. of propargyl diazo malonic esters)

RN 289673-95-6 HCAPLUS

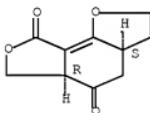
CN Furo[2,3-e]isobenzofuran-8(2H)-one, 3,6-dihydro- (CA INDEX NAME)



RN 289673-96-7 HCAPLUS

CN Furo[2,3-e]isobenzofuran-5,8-dione, 2,3,3a,4,5a,6-hexahydro-,
(3aR,5aS)-rel- (CA INDEX NAME)

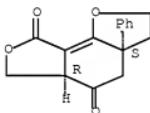
Relative stereochemistry.



RN 289673-97-8 HCAPLUS

CN Furo[2,3-e]isobenzofuran-5,8-dione, 2,3,3a,4,5a,6-hexahydro-3a-phenyl-,
(3aR,5aS)-rel- (CA INDEX NAME)

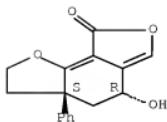
Relative stereochemistry.



RN 289673-98-9 HCAPLUS

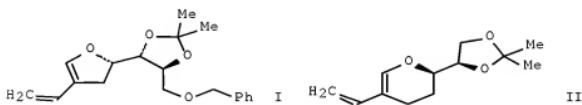
CN Furo[2,3-e]isobenzofuran-8(2H)-one,
3,3a,4,5-tetrahydro-5-hydroxy-3a-phenyl-, (3aR,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.



CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
 IT 289673-82-1P 289673-83-2P 289673-85-4P 289673-86-5P 289673-88-7P
 289673-89-8P 289673-90-1P 289673-93-4P 289673-95-6P
 289673-96-7P 289673-97-8P 289673-98-9P
 497070-65-2P 497070-69-6P 497070-70-9P 497070-71-0P 497070-72-1P
 497070-76-5P 497070-79-8P 497070-84-5P 497070-85-6P 497070-86-7P
 497070-95-8P 497070-96-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of polycyclic furans via rhodium catalyzed
 cyclization/Diels-Alder cycloaddn. of propargyl diazo malonic esters)
 REFERENCE COUNT: 97 THERE ARE 97 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 6 OF 19 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2002:938126 HCPLUS Full-text
 DOCUMENT NUMBER: 138:170042
 TITLE: A Facile Synthesis of Enantiopure Tricyclic Furanyl
 and Pyranyl Derivatives via Tungsten-Mediated
 Cycloalkenation and Diels-Alder Reaction
 AUTHOR(S): Huang, Heh-Lung; Liu, Rai-Shung
 CORPORATE SOURCE: Chemistry Department, National Tsing-Hua University,
 Hsinchu, Taiwan, Taiwan
 SOURCE: Journal of Organic Chemistry (2003), 68(3), 805-810
 CODEN: JOCSEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 138:170042
 GI



AB Chiral furanyl and pyranyl dienes I and II, bearing a chiral 1,3-dioxolane group which allows to control diastereoselective Diels-Alder reactions with electron-deficient olefins, were synthesized via cycloalkenylation of chiral tungsten alkynol complexes. Diels-Alder reactions of I and II with maleic anhydride, maleic imide, Ph maleimide, 1,4-benzoquinone, or 1,4-naphthoquinone gave stereoselectively the corresponding cycloadducts, which were further

converted into common tricyclic furanyl and pyranyl derivs. by degradation of chiral 1,3-dioxolane substituents into hydrogen atoms.

IT 496920-56-0 HCPLUS 496920-83-3P

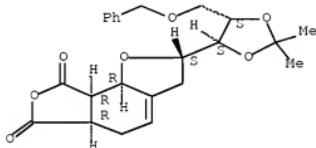
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of enantiopure tricyclic furanyl and pyranyl derivs. via tungsten-mediated cycloalkenylation and Diels-Alder reaction)

RN 496920-56-0 HCPLUS

CN Furo[2,3-e]isobenzofuran-6,8-dione,
2-[(4S,5S)-2,2-dimethyl-5-[(phenylmethoxy)methyl]-1,3-dioxolan-4-yl]-
2,3,5,5a,8a,8b-hexahydro-, (2S,5aR,8aR,8bR)- (CA INDEX NAME)

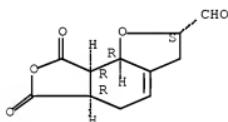
Absolute stereochemistry. Rotation (-).



RN 496920-83-3 HCPLUS

CN Furo[2,3-e]isobenzofuran-2-carboxaldehyde,
2,3,5,5a,6,8,8a,8b-octahydro-6,8-dioxo-, (2S,5aR,8aR,8bR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 496920-87-7P

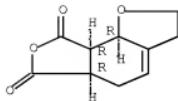
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of enantiopure tricyclic furanyl and pyranyl derivs. via tungsten-mediated cycloalkenylation and Diels-Alder reaction)

RN 496920-87-7 HCPLUS

CN Furo[2,3-e]isobenzofuran-6,8-dione, 2,3,5,5a,8a,8b-hexahydro-,
(5aR,8aR,8bR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



CC 27-13 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 29

IT 50622-09-8P 78513-03-8P 81028-12-8P 143360-25-2P 285565-67-5P
 496920-50-4P 496920-53-7P 496920-54-8P 496920-56-0P
 496920-58-2P 496920-60-6P 496920-62-8P 496920-71-9P 496920-73-1P
 496920-75-3P 496920-80-0P 496920-83-3P 496920-84-4P
 496920-85-5P 496920-92-4P 496920-94-6P 496920-96-8P 497064-88-7P
 497064-89-8P 497064-90-1P 497064-91-2P 497064-92-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of enantiopure tricyclic furanyl and pyranyl derivs. via tungsten-mediated cycloalkenylation and Diels-Alder reaction)

IT 496920-64-0P 496920-66-2P 496920-69-5P 496920-77-5P 496920-79-7P
 496920-82-2P 496920-87-7P 496920-89-9P 496920-91-3P
 496920-97-9P 496920-99-1P 496921-02-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of enantiopure tricyclic furanyl and pyranyl derivs. via tungsten-mediated cycloalkenylation and Diels-Alder reaction)

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 7 OF 19 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:856496 HCPLUS Full-text

DOCUMENT NUMBER: 138:152309

TITLE: Microbial transformation of mycophenolic acid. Part II

AUTHOR(S): Jekkel, A.; Barta, I.; Boros, S.; Suto, J.; Horvath, Gy.; Szabo, Zs.; Ambrus, G.

CORPORATE SOURCE: IVAX Drug Research Institute Ltd., Budapest, H-1045, Hung.

SOURCE: Journal of Molecular Catalysis B: Enzymatic (2002), 19-20, 209-214

CODEN: JMCBFB; ISSN: 1381-1177

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:152309

AB Bioconversion of mycophenolic acid (MPA, I) having considerable immuno-suppressant activity was attempted with a great number of microorganisms. Four *Streptomyces* strains were selected, which transformed MPA to various bioconversion products. These derivs. of MPA (II-VI) were isolated and their structures were determined by IR, 1H, 13C NMR and mass spectroscopic methods. In the course of bioconversions, mycophenolic acid underwent one or more of the following transformations: hydroxylation on the side chain or on the lactone ring, amide and alc. formation from the carboxylic acid group, oxidative cyclizations of the side chain and glycosylation.

IT 494922-54-5P

RL: BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or

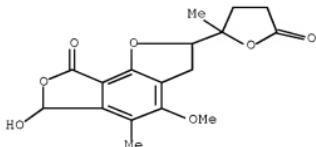
recovery); BIOL (Biological study); PREP (Preparation)

(microbial transformation of mycophenolic acid)

RN 494842-54-5 HCPLUS

CN Furo[2,3-*e*]isobenzofuran-8(2H)-one,
3,6-dihydro-6-hydroxy-4-methoxy-5-methyl-2-(tetrahydro-2-methyl-5-oxo-2-furanyl)- (CA INDEX NAME)

Currently available stereo shown.

CC 16-2 (Fermentation and Bioindustrial Chemistry)
IT 133538-73-5P 494841-99-5P 494842-52-3P 494842-54-5P

494842-57-8P

RL: BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(microbial transformation of mycophenolic acid)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 8 OF 19 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:769090 HCPLUS Full-text

DOCUMENT NUMBER: 138:255124

TITLE: Facile synthesis of enantiopure tricyclic furanyl derivatives via tungsten-mediated cycloalkenation reactions and Diels-Alder reactions

AUTHOR(S): Huang, Heh-Lung; Huang, Heh-Chang; Liu, Rai-Shung

CORPORATE SOURCE: Department of Chemistry, National Tsing Hua University, Hsinchu, Taichung, 30013, Taiwan

SOURCE: Tetrahedron Letters (2002), 43(44), 7983-7985
CODEN: TELEAY; ISSN: 0040-4039

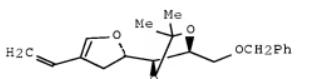
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:255124

GI



I

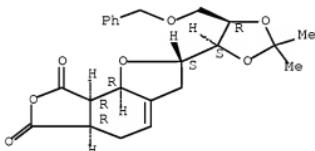
AB Chiral furanyl diene, (4*S*,5*R*)-4-[(2*S*)-4-ethenyl-2,3-dihydro-2-furanyl]-5-[(phenylmethoxy)methyl]-1,3-dioxolane (I), is easily prepared from cycloalkenation of chiral tungsten alkynol with acetaldehyde, followed by demetalation with Me3NO. This diene bears a chiral 1,3-dioxolane group to

control diastereoselective Diels-Alder reactions with electron-deficient olefins. The chiral 1,3-dioxolane substituent of the cycloadducts was degraded to a hydrogen atom to make these mols. possess a common furanyl functionality.

IT 502481-99-4P 502482-04-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (facile synthesis of enantiopure tricyclic furanyl derivs. via tungsten-mediated cycloalkenation and Diels-Alder reaction of (ethenylidihydrofuranyl)[(phenylmethoxy)methyl]dioxolane)

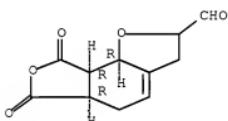
RN 502481-99-4 HCPLUS
 CN Furo[2,3-e]isobenzofuran-6,8-dione,
 2-[(4S,5R)-2,2-dimethyl-5-[(phenylmethoxy)methyl]-1,3-dioxolan-4-yl]-
 2,3,5,5a,8a,8b-hexahydro-, (2S,5aR,8aR,8bR)- (CA INDEX NAME)

Absolute stereochemistry.



RN 502482-04-4 HCPLUS
 CN Furo[2,3-e]isobenzofuran-2-carboxaldehyde,
 2,3,5,5a,6,8a,8b-octahydro-6,8-dioxo-, (5aR,8aR,8bR)- (CA INDEX NAME)

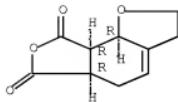
Absolute stereochemistry.



IT 496920-87-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (facile synthesis of enantiopure tricyclic furanyl derivs. via tungsten-mediated cycloalkenation and Diels-Alder reaction of (ethenylidihydrofuranyl)[(phenylmethoxy)methyl]dioxolane)

RN 496920-87-7 HCPLUS
 CN Furo[2,3-e]isobenzofuran-6,8-dione, 2,3,5,5a,8a,8b-hexahydro-, (5aR,8aR,8bR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 27
 IT 55904-12-6P 81801-08-3P 502481-96-1P 502481-97-2P 502481-98-3P
 502481-99-4P 502482-00-0P 502482-01-1P 502482-04-4P
 502482-05-5P 502482-06-6P 502613-15-2P 502613-36-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (facile synthesis of enantiopure tricyclic furanyl derivs. via
 tungsten-mediated cycloalkenation and Diels-Alder reaction of
 (ethenylidihydrofuranyl)[(phenylmethoxy)methyl]dioxolane)
 IT 496920-97-7P 496920-89-9P 496920-91-3P 502482-02-2P
 502482-03-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (facile synthesis of enantiopure tricyclic furanyl derivs. via
 tungsten-mediated cycloalkenation and Diels-Alder reaction of
 (ethenylidihydrofuranyl)[(phenylmethoxy)methyl]dioxolane)
 REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 9 OF 19 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2002:14876 HCPLUS Full-text
 DOCUMENT NUMBER: 136:216986
 TITLE: Novel Mycophenolic Adenine Bis(phosphonate) Analogues
 As Potential Differentiation Agents against Human
 Leukemia
 AUTHOR(S): Pankiewicz, Krzysztof W.; Lesiak-Watanabe, Krystyna
 B.; Watanabe, Kyoichi A.; Patterson, Steven E.;
 Jayaram, Hirenagalur N.; Yalowitz, Joel A.; Miller,
 Michael D.; Seidman, Michael; Majumdar, Alokes;
 Prehna, Gerd; Goldstein, Barry M.
 CORPORATE SOURCE: Pharmasset Inc., Tucker, GA, 30084, USA
 SOURCE: Journal of Medicinal Chemistry (2002), 45(3), 703-712
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:216986
 AB Novel mycophenolic adenine dinucleotide (MAD) analogs have been prepared as potential inhibitors of inosine monophosphate dehydrogenase (IMPDH). MAD analogs resemble NAD binding at the cofactor binding domain of IMPDH; however, they cannot participate in hydride transfer and therefore inhibit the enzyme. The methylenebis(phosphonate) analogs C2-MAD and C4-MAD were obtained by coupling 2',3'-O-isopropylideneadenosine 5'-methylenebis(phosphonate) with mycophenolic alcs. in the presence of diisopropylcarbodiimide followed by deprotection. C2-MAD and C4-MAD were found to inhibit the growth of K562 cells ($IC_{50} = 0.7 \mu M$ and $IC_{50} = 0.1 \mu M$, resp.) as potently as mycophenolic acid ($IC_{50} = 0.3 \mu M$). In addition, C2-MAD and C4-MAD triggered vigorous differentiation of K562 cells an order of magnitude more potently than tiazofurin, and MAD analogs were resistant to glucuronidation in vitro. These

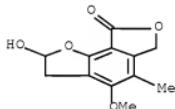
results show that C2-MAD and C4-MAD may be of therapeutic interest in the treatment of human leukemias.

IT 402731-00-4P

RL: BPN (Biosynthetic preparation); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of mycophenolic adenine bisphosphonate analogs as potential differentiation agents against human leukemia)

RN 402731-00-4 HCPLUS

CN Euro[2,3-e]isobenzofuran-8(2H)-one,
3,6-dihydro-2-hydroxy-4-methoxy-5-methyl- (CA INDEX NAME)



CC 33-9 (Carbohydrates)

Section cross-reference(s): 1, 7

IT 402731-00-4P

RL: BPN (Biosynthetic preparation); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of mycophenolic adenine bisphosphonate analogs as potential differentiation agents against human leukemia)

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 10 OF 19 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:396982 HCPLUS Full-text

DOCUMENT NUMBER: 133:193098

TITLE: Facile Construction of Novel Polycyclic Ring Systems Using a Metallocarbonyl-Induced Cyclization of Acetylenic Diazo Carbonyl Compounds

AUTHOR(S): Padwa, Albert; Straub, Christopher S.

CORPORATE SOURCE: Department of Chemistry, Emory University, Atlanta, GA, 30322, USA

SOURCE: Organic Letters (2000), 2(14), 2093-2095
CODEN: ORLE7; ISSN: 1523-7060

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:193098

AB The Rh(II)-catalyzed reactions of diazo 2-propynylmalonamic acid ester derivs. produce furo[3,4-c]furans in excellent yield. The methodol. was applied to the synthesis of several polycyclic systems by first generating a 2-alkoxy-substituted furan and then allowing it to undergo a subsequent intramol. Diels-Alder cycloaddn. Ring opening of the resulting cycloadduct is followed by deprotonation to furnish a rearranged keto lactone.

IT 289673-95-6P 289673-96-7P 289673-97-8P

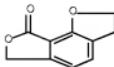
289673-98-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of polycyclic rings via Rh(II)-catalyzed IMDAF cascade of diazomalonate esters)

RN 289673-95-6 HCPLUS

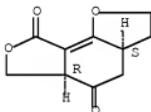
CN Furo[2,3-e]isobenzofuran-8(2H)-one, 3,6-dihydro- (CA INDEX NAME)



RN 289673-96-7 HCAPLUS

CN Furo[2,3-e]isobenzofuran-5,8-dione, 2,3,3a,4,5a,6-hexahydro-, (3aR,5aS)-rel- (CA INDEX NAME)

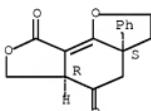
Relative stereochemistry.



RN 289673-97-8 HCAPLUS

CN Furo[2,3-e]isobenzofuran-5,8-dione, 2,3,3a,4,5a,6-hexahydro-3a-phenyl-, (3aR,5aS)-rel- (CA INDEX NAME)

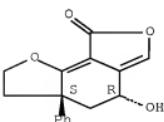
Relative stereochemistry.



RN 289673-98-9 HCAPLUS

CN Furo[2,3-e]isobenzofuran-8(2H)-one, 3,3a,4,5-tetrahydro-5-hydroxy-3a-phenyl-, (3aR,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.



CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 27

IT 289673-85-4P 289673-86-5P 289673-88-7P 289673-89-8P 289673-90-1P
 289673-95-6P 289673-96-7P 289673-97-8P
 289673-98-9P 289674-00-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of polycyclic rings via Rh(II)-catalyzed IMDAF cascade of diazomalonate esters)

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 11 OF 19 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2000:338368 HCPLUS Full-text
 DOCUMENT NUMBER: 133:135199
 TITLE: Facile Synthesis of Oxa- and Azacyclic Dienes via Cycloalkenation of Alkynyltungsten Compounds. Stereoselective Construction of Tricyclic Furan and Pyran Derivatives via Intramolecular Diels-Alder Reaction

AUTHOR(S): Li, Wen-Tai; Pan, Min-Hui; Wu, Yi-Ru; Wang, Sue-Lein; Liao, Fen-Lin; Liu, Rai-Shung

CORPORATE SOURCE: Department of Chemistry, National Tsing-Hua University, Hsinchu, Taiwan

SOURCE: Journal of Organic Chemistry (2000), 65(12), 3761-3766
 CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

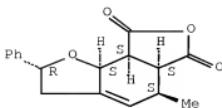
OTHER SOURCE(S): CASREACT 133:135199

AB A convenient and short synthesis of functionalized oxacyclic and azacyclic dienes is developed on the basis of organotungsten chemical Alkynyltungsten compds. bearing a tethered alc. and amine are treated with aldehydes and BF₃.Et₂O in cold di-Et ether to give tungsten-heterocyclic carbenium salts, further leading to tungsten-heterocyclic dienes via deprotonation with Et₃N. Hydrodemetalation of these tungsten-heterocyclic dienes is performed by the action of anhydrous Me₃NO in MeCN. This method is applicable to the synthesis of a number of oxa- and azacyclic dienes, including those tethered with an electron-deficient olefin. The oxacyclic 1,3,8-nonatrienes and 1,3,9-decatrienes undergo intramol. Diels-Alder reactions upon heating in toluene, yielding tricyclic tetrahydropyran and -furan derivs. with excellent diastereoselectivities.

IT 285565-50-6P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (stereoselective preparation of tricyclic furans and pyran via cycloalkenation of alkynyltungsten compds. and intramol. Diels-Alder reaction)

RN 285565-50-6 HCPLUS
 CN Furo[2,3-e]isobenzofuran-6,8-dione,
 2,3,5,5a,8a,8b-hexahydro-5-methyl-2-phenyl-, (2R,5S,5aS,8aS,8bS)-rel- (CA INDEX NAME)

Relative stereochemistry.



CC 27-14 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 29

IT 285565-50-6P 285565-61-9P 285565-62-0P 285565-63-1P

285565-64-2P 285565-65-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of tricyclic furans and pyran via
cycloalkenation of alkynyltungsten compds. and intramol. Diels-Alder
reaction)

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 12 OF 19 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:153126 HCPLUS Full-text

DOCUMENT NUMBER: 130:342877

TITLE: Degradation products of mycophenolate mofetil in aqueous solution

AUTHOR(S): Hooijmaijer, Elvira; Brandl, Michael; Nelson, Janis;
Lustig, David

CORPORATE SOURCE: Roche Bioscience, Palo Alto, CA, 94304, USA

SOURCE: Drug Development and Industrial Pharmacy (1999),
25(3), 361-365

CODEN: DDIPD8; ISSN: 0363-9045

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The thermal and peroxide-catalyzed degradation products of mycophenolate mofetil (I) were studied in aqueous solution at pH 2.0, 3.5, 6.0, and 8.2. The major thermal degradation product of I observed was mycophenolic acid (II). At pH 6.0 and 8.2, II was the only product observed in the absence of peroxide, while at pH 2.0 and 3.5, the lactone analog of mycophenolic acid, a hydroxy lactone due to oxygenation of the double bond, and an unidentified product were formed. The hydroxy lactone degraded to 4-hydroxy-6-methoxy-7-methyl-3-oxo-1,3-dihydroisobenzofuran-5-carbaldehyde on prolonged storage and was present in the sample stressed at pH 2. II, the N-oxide of mycophenolate mofetil, the hydroxy lactone of mycophenolic acid, and the erythro form of 4-methoxy-5-methyl-2-(2-methyl-5-oxotetrahydrofuran-2-yl)-3,6-dihydro-2H-1,7-dioxa-as-indacen-8-one were observed in the presence of hydrogen peroxide at pH 3.5, 6.0, and 8.2. In addition, at pH 8.2, 4-hydroxy-4-(4-methoxy-5-methyl-8-oxo-2,3,6,8-tetrahydro-1,7-dioxa-as-indacen-2-yl)pentanoic acid was seen. Peroxide-stressed samples at pH 2.0 gave no major degradation peaks, but a small amount of the hydroxy lactone of mycophenolic acid was formed.

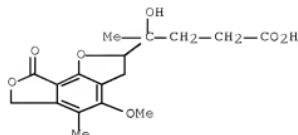
IT 224052-52-2 224052-53-3

RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(degradation products of mycophenolate mofetil in aqueous solution)

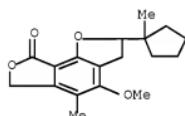
RN 224052-52-2 HCPLUS

CN Furo[2,3-*e*]isobenzofuran-2-butanoic acid,

2,3,6,8-tetrahydro-*y*-hydroxy-4-methoxy-*y*,5-dimethyl-8-oxo-
(CA INDEX NAME)



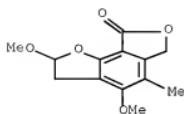
RN 224052-53-3 HCAPLUS
 CN Furo[2,3-e]isobenzofuran-8(2H)-one,
 3,6-dihydro-4-methoxy-5-methyl-2-(1-methylcyclopentyl)- (CA INDEX NAME)



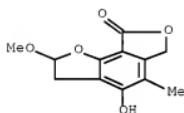
CC 63-5 (Pharmaceuticals)
 Section cross-reference(s): 22
 IT 622-40-2, 4-Morpholineethanol 24280-93-1, Mycophenolic acid 26644-06-4
 26675-76-3 67549-56-8 224052-51-1 224052-52-2
 224052-53-3
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
 (degradation products of mycophenolate mofetil in aqueous solution)
 REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L20 ANSWER 13 OF 19 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1997:476714 HCAPLUS Full-text
 DOCUMENT NUMBER: 127:149019
 ORIGINAL REFERENCE NO.: 127:28789a,28792a
 TITLE: Total synthesis of mycophenolic acid
 AUTHOR(S): de la Cruz, Ricardo A.; Talamas, Francisco X.;
 Vazquez, Alfredo; Muchowski, Joseph M.
 CORPORATE SOURCE: Syntex S. A. de C. V., Div. de Investigacion, Morelos,
 62500, Mex.
 SOURCE: Canadian Journal of Chemistry (1997), 75(6), 641-645
 CODEN: CJCHAG; ISSN: 0008-4042
 PUBLISHER: National Research Council of Canada
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 127:149019
 AB A total synthesis of mycophenolic acid is reported. Diels-Alder reaction of
 [5-methoxy-3-(1-methoxypropenyl)-4,5-dihydrofuran-2-yloxy]- trimethylsilylane
 with 3-benzenesulfinyl-5H-furan-2-one afforded the hexasubstituted nucleus.
 The side chain was constructed from the unveiled aldehyde.
 IT 193277-77-9P 193277-88-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

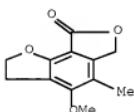
(total synthesis of mycophenolic acid)
 RN 193277-77-9 HCPLUS
 CN Furo[2,3-e]isobenzofuran-8(2H)-one, 3,6-dihydro-2,4-dimethoxy-5-methyl-
 (CA INDEX NAME)



RN 193277-88-2 HCPLUS
 CN Furo[2,3-e]isobenzofuran-8(2H)-one,
 3,6-dihydro-4-hydroxy-2-methoxy-5-methyl- (CA INDEX NAME)



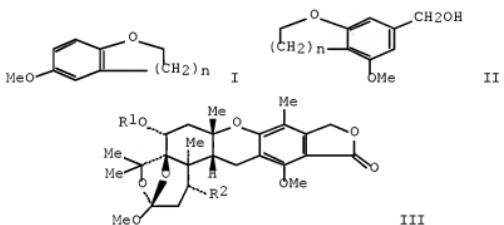
IT 193277-83-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (total synthesis of mycophenolic acid)
 RN 193277-83-7 HCPLUS
 CN Furo[2,3-e]isobenzofuran-8(2H)-one, 3,6-dihydro-4-methoxy-5-methyl- (CA INDEX NAME)



CC 26-6 (Biomolecules and Their Synthetic Analogs)
 IT 13312-25-9P 24953-96-6P 57061-31-1P 138768-41-9P 172151-14-3P
 193277-70-2P 193277-73-5P 193277-75-7P 193277-77-9P
 193277-79-1P 193277-81-5P 193277-85-9P 193277-89-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (total synthesis of mycophenolic acid)
 IT 24280-93-1P, Mycophenolic acid 193277-83-7P
 RL: SPN (Synthetic preparation); PRBP (Preparation)
 (total synthesis of mycophenolic acid)

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT.

L20 ANSWER 14 OF 19 HCPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:483671 HCPLUS Full-text
DOCUMENT NUMBER: 121:83671
ORIGINAL REFERENCE NO.: 121:15053a,15056a
TITLE: Relevance of Conformational Constraints to the
Regioselective Lithiation of Aromatic Diethers.
Application to the Convenient Construction of the DEF
Tricyclic Subunit of the Australides
AUTHOR(S): Paquette, Leo A.; Schulze, Matthias M.; Bolin, David
G.
CORPORATE SOURCE: Evans Chemical Laboratories, Ohio State University,
Columbus, OH, 43210, USA
SOURCE: Journal of Organic Chemistry (1994), 59(8), 2043-51
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:83671
GI

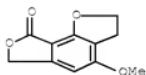


AB The lithiation of I ($n = 1, 2$) is shown to occur at all three sites with a dissimilar kinetic preference. For the dihydrofuran, reaction at the proton labeled $H\beta'$ operates predominantly; in the dihydropyran example, $H\alpha$ is the favored site of deprotonation. These protons represent those that are the most deshielded in the resp. ^{1}H -NMR spectra. The same is true for II ($n = 1, 2$), both of which undergo metalation adjacent to the ring oxygen. No crossover in regioselectivity is observed, presumably because the methoxy substituent is sterically precluded from rotating freely. Mixed complexes (dimers, etc.) or mixed aggregates in low equilibrium concentration are key to understanding the acidification phenomenon of ortho hydrogens. As a consequence of the dominance of regiocontrol by the ring oxygen in II ($n = 2$), a convenient means has been developed for elaboration of the tricyclic eastern sector of the austalide mycotoxins, III [R1 = Ac, R2 = H (A); R1 = R2 = H (B); R1 = Ac, R2 = OAc (C); R1 = H, R2 = OAc (D); R1 = Ac, R2 = OH (E); R1 = H, R2 = OH (F)].

IT 156297-74-4E

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, regioselectivity in)
 RN 156297-74-4 HCAPLUS
 CN Furo[2,3-e]isobenzofuran-8(2H)-one, 3,6-dihydro-4-methoxy- (CA INDEX
 NAME)



CC 30-25 (Terpenes and Terpenoids)
 IT 99355-75-6P 99385-73-6P 99385-74-7P 99385-75-8P 152188-40-4P
 152188-41-5P 152188-42-6P 152188-47-1P 152188-48-2P 152188-49-3P
 152188-50-6P 156297-74-4P 156297-75-5P 156297-76-6P
 156297-77-7P 156297-78-8P 156297-79-9P 156297-80-2P 156297-81-3P
 156297-82-4P 156297-83-5P 156297-84-6P 156297-85-7P 156297-86-8P
 156297-87-9P 156297-88-0P 156297-89-1P 156297-90-4P 156297-91-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, regioselectivity in)

L20 ANSWER 15 OF 19 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1987:423262 HCAPLUS Full-text
 DOCUMENT NUMBER: 107:23262
 ORIGINAL REFERENCE NO.: 107:3931a,3934a
 TITLE: Preparation of 5-alkyl- and
 5-arylalkyl-2-methylbenzofuran-6,7-dicarboxylic acids.
 Conversion of 5-arylalkylbenzofuran anhydrides to new
 heterocycles
 AUTHOR(S): Cabares, Jacques; Mavoungou-Gomes, Louis
 CORPORATE SOURCE: Lab. Chim. Org., UER Sci. Med. Pharm., Angers, 49045,
 Fr.
 SOURCE: Bulletin de la Societe Chimique de France (1986), (3),
 401-12
 CODEN: BSCFAS; ISSN: 0037-8968
 DOCUMENT TYPE:
 LANGUAGE:
 OTHER SOURCE(S): CASREACT 107:23262
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

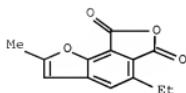
AB Diels-Alder reaction of 5-alkyl-2-acetonylfurans (I; R = Me, Et, PhCH₂CH₂, etc.) with MeO₂C.tplbond.CCO₂Me gave oxabicycloheptadienedicarboxylates II (same R). Treating II with BF₃.OEt₂ gave benzofuranedicarboxylates III (or their anhydrides or acids). Cyclization reactions of these benzofuranedicarboxylate derivs. gave polycyclic benzofuran derivs. Thus, cyclization of III (R = Me) with NH₂NH₂ gave the euporphthalazinedione IV. Among the other polycyclic compds. prepared were the anthrafurancarboxylic acid derivative V and the benzocycloheptafurotriazolophthalazine derivs. VI.
 IT 73606-75-4P 73606-76-5P 73606-77-6P
 108604-53-1P 108604-54-2P 108604-55-3P
 108604-56-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and reactions of)

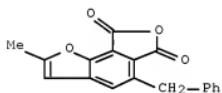
RN 73606-75-4 HCPLUS

CN Furo[2,3-e]isobenzofuran-6,8-dione, 5-ethyl-2-methyl- (CA INDEX NAME)



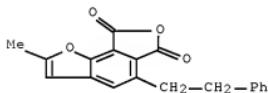
RN 73606-76-5 HCPLUS

CN Furo[2,3-e]isobenzofuran-6,8-dione, 2-methyl-5-(phenylmethyl)- (CA INDEX NAME)



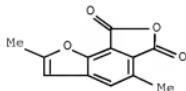
RN 73606-77-6 HCPLUS

CN Furo[2,3-e]isobenzofuran-6,8-dione, 2-methyl-5-(2-phenylethyl)- (CA INDEX NAME)



RN 108604-53-1 HCPLUS

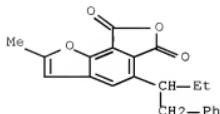
CN Furo[2,3-e]isobenzofuran-6,8-dione, 2,5-dimethyl- (CA INDEX NAME)



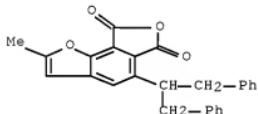
RN 108604-54-2 HCPLUS

CN Furo[2,3-e]isobenzofuran-6,8-dione, 2-methyl-5-[1-(phenylmethyl)propyl]-

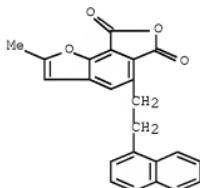
(CA INDEX NAME)



RN 108604-55-3 HCAPLUS

CN Furo[2,3-e]isobenzofuran-6,8-dione,
2-methyl-5-[2-phenyl-1-(phenylmethyl)ethyl]- (CA INDEX NAME)

RN 108604-56-4 HCAPLUS

CN Furo[2,3-e]isobenzofuran-6,8-dione, 2-methyl-5-[2-(1-naphthalenyl)ethyl]-
(CA INDEX NAME)

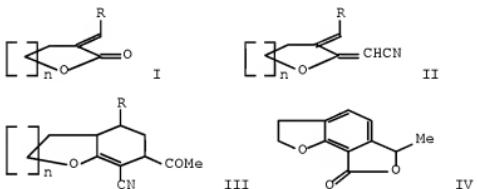
CC 28-1 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 27

IT 68654-70-6P 73606-75-4P 73606-76-5P
 73606-77-6P 73606-81-2P 73606-82-3P 73606-85-6P
 73606-87-8P 73606-93-6P 108604-52-0P 108604-53-1P
 108604-54-2P 108604-55-3P 108604-56-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reactions of)

L20 ANSWER 16 OF 19 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:101992 HCPLUS Full-text
 DOCUMENT NUMBER: 106:101992
 ORIGINAL REFERENCE NO.: 106:16699a,16702a
 TITLE: Novel dienes from α -ylidene and
 α -alkoxylidene lactones. Useful intermediates
 for the synthesis of benzofurans
 AUTHOR(S): Murray, Alistair W.; Murray, Neil D.; Reid, Robert G.
 CORPORATE SOURCE: Dep. Chem., Univ. Dundee, Dundee, DD1 4HN, UK
 SOURCE: Journal of the Chemical Society, Chemical
 Communications (1986), (16), 1230-2
 DOCUMENT TYPE: CODEN: JCCCAT; ISSN: 0022-4936
 LANGUAGE: Journal
 English
 OTHER SOURCE(S): CASREACT 106:101992
 GI



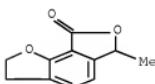
AB Reaction of lactones I ($R = H, Et, Ph, OMe, OEt, n = 1; R = Ph, n = 2$) with BuLi and MeCN in THF at $-78^\circ C$ for 3 h gave mixts. of (Z)- and (E)-dienes II (R, n as before). Reaction of II with MeCOCH₂:CH₂ gave the tetrahydrobenzofuran III in 23-40% overall yield from I. III ($R = H, n = 1$) was converted to benzofuranolactone IV in 3 steps.

IT 106895-67-42

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 106895-67-4 HCAPLUS

CN Euro[2,3-e]isobenzofuran-8(2H)-one, 3,6-dihydro-6-methyl- (CA INDEX NAME)



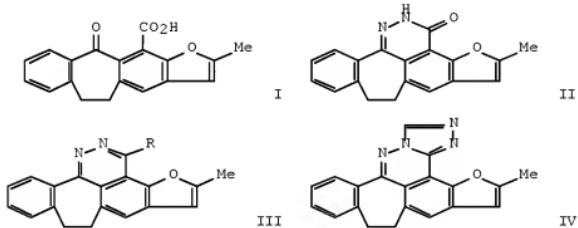
CC 27-7 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 23

IT 106895-60-7P 106895-61-8P 106895-62-9P 106895-63-0P 106895-64-1P

RL: SPN (Synthetic preparation); PREP (Preparation (preparation of))

L20 ANSWER 17 OF 19 HCPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1980:198336 HCPLUS Full-text
DOCUMENT NUMBER: 92:198336
ORIGINAL REFERENCE NO.: 92:32131a,32134a
TITLE: Preparation of 6,7-dicarboxybenzofurans and
application to the synthesis of new heterocyclics
AUTHOR(S): Cabares, Jacques; Gomes, Louis Mavoungou
CORPORATE SOURCE: Lab. Chim. Org., Unites Enseign. Rech. Sci. Med.
Pharm., Angers, 49000, Fr.
SOURCE: Comptes Rendus des Seances de l'Academie des Sciences,
Serie C: Sciences Chimiques (1979), 289(12), 321-4
DOCUMENT TYPE: CODEN: CHDCAQ; ISSN: 0567-6541
LANGUAGE: Journal
OTHER SOURCE(S): French
GI: CASREACT 92:198336

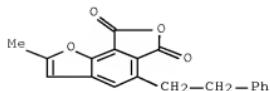


AB The γ -oxo acid I, which was prepared by the cyclocondensation of 2-methyl-5-phenethyl-6,7-benzo furandicarboxylic anhydride, was converted to fused phthalazinone II. I was treated with N_2H_4 to yield II, which was treated with POC13 to give III ($\text{R} = \text{Cl}$), which was treated with N_2H_4 to give III ($\text{R} = \text{NNH}_2$). The latter reacted with HC(OEt)_3 to give triazolophthalazine IV.

IT 73606-77-6P 73606-80-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation reaction of)

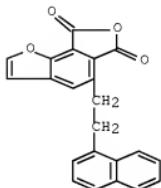
BN 73606-77-6 HCAPLUS

CN Furo[2,3-e]isobenzofuran-6,8-dione, 2-methyl-5-(2-phenylethyl)- (CA INDEX NAME)



RN 73606-80-1 HCAPLUS

CN Furo[2,3-e]isobenzofuran-6,8-dione, 5-[2-(1-naphthalenyl)ethyl]- (CA INDEX NAME)



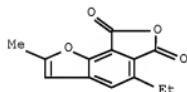
IT 73606-75-4P 73606-76-5P 73606-78-7P

73606-79-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

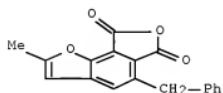
RN 73606-75-4 HCAPLUS

CN Furo[2,3-e]isobenzofuran-6,8-dione, 5-ethyl-2-methyl- (CA INDEX NAME)



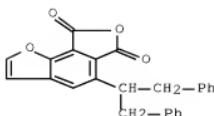
RN 73606-76-5 HCAPLUS

CN Furo[2,3-e]isobenzofuran-6,8-dione, 2-methyl-5-(phenylmethyl)- (CA INDEX NAME)

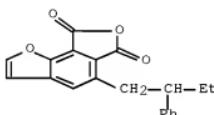


RN 73606-78-7 HCAPLUS

CN Furo[2,3-e]isobenzofuran-6,8-dione, 5-[2-phenyl-1-(phenylmethyl)ethyl]- (CA INDEX NAME)

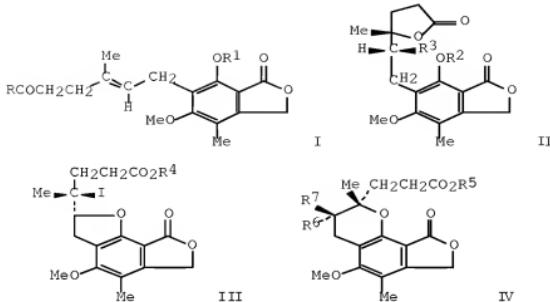


RN 73606-79-8 HCPLUS
 CN Furo[2,3-e]isobenzofuran-6,8-dione, 5-(2-phenylbutyl)- (CA INDEX NAME)



CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 27
 IT 73606-77-6P 73606-80-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and cyclocondensation reaction of)
 IT 73606-75-4P 73606-76-5P 73606-78-7P
 73606-79-3P 73606-86-7P 73606-88-9P 73606-89-0P
 73606-90-3P 73606-94-7P 73606-95-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

L20 ANSWER 18 OF 19 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1978:170004 HCPLUS Full-text
 DOCUMENT NUMBER: 88:170004
 ORIGINAL REFERENCE NO.: 88:26795a,26798a
 TITLE: Derivatives of mycophenolic acid
 AUTHOR(S): Carman, Raymond M.
 CORPORATE SOURCE: Dep. Chem., Univ. Queensland, St. Lucia, Australia
 SOURCE: Australian Journal of Chemistry (1978), 31(2), 353-64
 CODEN: AJCHAS; ISSN: 0004-9425
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB About 22 mycophenolic and mycochromenic acid derivs. I-IV (R = OH, OMe, n-octyloxy, n-octylamino; R1, R2 = H, Ac; R3, R7 = H, Br, I; R4 = H, Me; R5 = H, Me, Et; R6 = H, I) were prepared and their structures determined according to their NMR spectra.

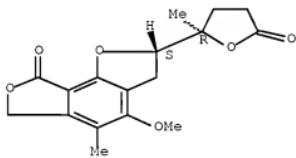
IT 66342-04-9

RL: PRP (Properties)
(NMR of)

RN 66342-04-9 HCAPLUS

CN Furo[2,3-*e*]isobenzofuran-8(2H)-one,
3,6-dihydro-4-methoxy-5-methyl-2-[(2*R*)-tetrahydro-2-methyl-5-oxo-2-furanyl]-, (2*S*)-rel- (CA INDEX NAME)

Relative stereochemistry.



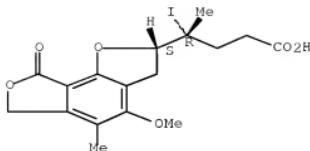
IT 66341-95-5P 66341-96-6P 66342-02-7P
66342-09-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 66341-95-5 HCAPLUS

CN Benzo[2,1-*b*:3,4-*c*']difuran-2-butanoic acid,
(γ R,2*S*)-rel- (CA INDEX NAME)

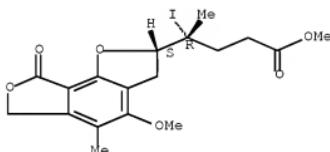
Relative stereochemistry.



RN 66341-96-6 HCPLUS

CN Benzo[2,1-b:3,4-c']difuran-2-butanoic acid,
2,3,6,8-tetrahydro- γ -iodo-4-methoxy- γ ,5-dimethyl-8-oxo-,
methyl ester, (γ R,2S)-rel- (CA INDEX NAME)

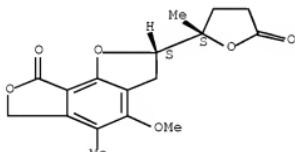
Relative stereochemistry.



RN 66342-02-7 HCPLUS

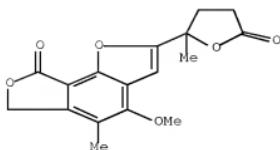
CN Furo[2,3-e]isobenzofuran-8(2H)-one,
3,6-dihydro-4-methoxy-5-methyl-2-[(2R)-tetrahydro-2-methyl-5-oxo-2-
furanyl]-, (2R)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 66342-09-4 HCPLUS

CN Furo[2,3-e]isobenzofuran-8(6H)-one,
4-methoxy-5-methyl-2-(tetrahydro-2-methyl-5-oxo-2-furanyl)- (CA INDEX
NAME)



CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))
 IT 66342-03-8 66342-04-9 66342-05-0 66342-06-1 66342-07-2
 66342-08-3

RL: PRP (Properties)
 (NMR of)

IT 24243-38-7P 31858-66-9P 66341-84-2P 66341-85-3P 66341-86-4P
 66341-88-6P 66341-89-7P 66341-90-0P 66341-93-3P 66341-95-5P
 66341-96-6P 66341-98-8P 66341-99-9P 66342-01-6P
 66342-02-7P 66342-03-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

L20 ANSWER 19 OF 19 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1970:484854 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 73:84854

ORIGINAL REFERENCE NO.: 73:13855a,13858a

TITLE: Microbial modification of mycophenolic acid

AUTHOR(S): Jones, Derrick Fleet; Moore, Ronald Haywood; Crawley, G. C.

CORPORATE SOURCE: Pharm. Div., Imp. Chem. Ind. Ltd., Macclesfield, UK

SOURCE: Journal of the Chemical Society [Section] C: Organic (1970), (12), 1725-37

CODEN: JSOOAX; ISSN: 0022-4952

DOCUMENT TYPE: Journal

LANGUAGE: English

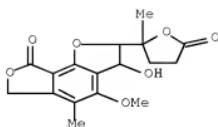
AB On incubation with selected microorganisms mycophenolic acid underwent one or more of the following transformations: (a) oxygenation of the 4-Me group, (b) oxygenation of the 3'-Me group and lactonization, (c) oxidation at C-3, (d) loss of the double bond and oxidation at C-4', (e) oxygenation of the double bond, (f) oxygenation and cyclization of the terpenoid substituent, (g) oxidative cyclization of the terpenoid substituent and (h) combination of the carboxy group with the amino groups of glycine and alanine. The structures of the fermentation products were established by spectroscopic methods. The biogenesis of the fermentation products is discussed and some preps. of cyclic ethers from mycophenolic acid derivs. are described.

IT 26644-09-6 26644-09-7 26644-12-2

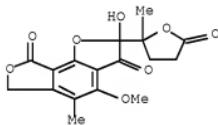
RL: FORM (Formation, nonpreparative)
 (formation of, from mycophenolic acid by microorganisms)

RN 26644-08-6 HCAPLUS

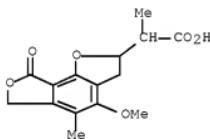
CN Furo[2,3-e]isobenzofuran-8(2H)-one,
 3,6-dihydro-3-hydroxy-4-methoxy-5-methyl-2-(tetrahydro-2-methyl-5-oxo-2-furanyl)- (CA INDEX NAME)



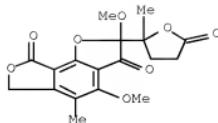
RN 26644-09-7 HCPLUS
 CN Furo[2,3-e]isobenzofuran-3,8(2H,6H)-dione,
 2-hydroxy-4-methoxy-5-methyl-2-(tetrahydro-2-methyl-5-oxo-2-furanyl)- (CA INDEX NAME)



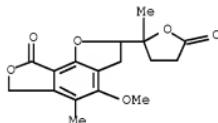
RN 26644-12-2 HCPLUS
 CN Furo[2,3-e]isobenzofuran-2-acetic acid,
 2,3,6,8-tetrahydro-4-methoxy- α ,5-dimethyl-8-oxo- (CA INDEX NAME)



IT 26644-10-0P 26693-54-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 26644-10-0 HCPLUS
 CN Furo[2,3-e]isobenzofuran-3,8(2H,6H)-dione,
 2,4-dimethoxy-5-methyl-2-(tetrahydro-2-methyl-5-oxo-2-furanyl)- (CA INDEX NAME)



RN 26693-54-9 HCAPLUS
 CN Furo[2,3-*e*]isobenzofuran-8(2H)-one,
 3,6-dihydro-4-methoxy-5-methyl-2-(tetrahydro-2-methyl-5-oxo-2-furanyl)-
 (CA INDEX NAME)



CC 8 (Microbial Biochemistry)
 IT 26644-01-9 26644-02-0 26644-03-1 26644-06-4 26644-07-5
 26644-09-6 26644-09-7 26644-12-2 26644-15-5
 26644-17-7 26644-26-8 26644-28-0 26644-31-5 26644-33-7
 26644-34-8 26675-76-3 26675-77-4 26840-17-5 30891-96-4
 RL: FORM (Formation, nonpreparative)
 (formation of, from mycophenolic acid by microorganisms)
 IT 26644-04-2P 26644-05-3P 26644-10-0P 26644-11-1P
 26644-13-3P 26644-16-6P 26644-18-8P 26644-19-9P 26644-20-2P
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 26644-27-9P 26644-29-1P 26644-30-4P 26644-32-6P 26644-35-9P
 26644-36-0P 26644-37-1P 26644-38-2P 26644-39-3P 26644-40-6P
 26644-41-7P 26675-78-5P 26675-79-6P 26675-80-9P 26675-81-0P
 26675-82-1P 26693-44-7P 26693-45-8P 26693-46-9P 26693-53-8P
 26693-54-9P 26853-35-0P 26853-36-1P 26853-37-2P
 26853-38-3P 26853-43-0P 26853-44-1P 26853-45-2P 26853-54-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

10/576758

***** SEARCH HISTORY *****

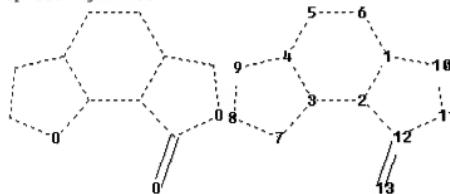
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FILE 'REGISTRY' ENTERED AT 10:58:57 ON 12 DEC 2008

L1 STRUCTURE UPLOADED
D

Uploading L1.str



chain nodes :

13

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

12-13

ring bonds :

1-2 1-6 1-10 2-3 2-12 3-4 3-7 4-5 4-9 5-6 7-8 8-9 10-11 11-12

exact/norm bonds :

1-2 1-6 1-10 2-3 2-12 3-4 3-7 4-5 4-9 5-6 7-8 8-9 10-11 11-12 12-13

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:CLASS

L2 4 SEA SSS SAM L1
D SCAN

L3 52 SEA SSS FUL L1
SAVE TEM L3 COV758REGL1/A

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L4 22 SEA ABB=ON PLU=ON L3

L5 5 SEA ABB=ON PLU=ON L4 AND PHARMAC?/SC, SX

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L6 1 SEA ABB=ON PLU=ON 850078-65-8/RN

D SCAN

L7 1 SEA ABB=ON PLU=ON 66341-91-1/RN

D SCAN

10/576758

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L9 1 SEA ABB=ON PLU=ON L4 AND L8

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D SCAN

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L11 6 SEA ABB=ON PLU=ON L4 AND 26/SC,SX
L12 50007 SEA ABB=ON PLU=ON LIU J?/AU
L13 12465 SEA ABB=ON PLU=ON ZHENG Y?/AU
L14 2276 SEA ABB=ON PLU=ON QIN X?/AU
L15 15784 SEA ABB=ON PLU=ON YANG L?/AU
L16 3525 SEA ABB=ON PLU=ON DONG Z?/AU
L17 15567 SEA ABB=ON PLU=ON WANG R?/AU
L18 3211 SEA ABB=ON PLU=ON TAN J?/AU
L19 3 SEA ABB=ON PLU=ON (((L12 OR L13 OR L14 OR L15 OR L16 OR L17
OR L18)) AND L4) OR (L4 AND L8)
L20 19 SEA ABB=ON PLU=ON L4 NOT L19
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SAVE TEMP L20 COV758HCAP/A

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D L19 1-3 IBIB ABS HITSTR

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D QUE L20

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D L20 1-19 IBIB ABS HITSTR HITIND

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